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Slow-Neutron Scattering by Rotators. II

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The methods developed in a previous paper for extending the neutron scattering formalism of Zemach and Glauber to any type of molecular rotator have been employed to derive generalized forms of the differential cross sections for rotator scattering. A mass-ratio expansion for the treatment of the high-energy limit is illustrated on the classical cross section and then employed in the treatment of the more general quantum-mechanical expression for the differential cross section. The results apply to an arbitrarily asymmetric rotator. The very low energy approximation is carried out for the symmetric rotator, and the procedure is compared with the explicit summing of the partial cross sections for individual rotational transitions. The inelastic correction to the static approximation for interference scattering is calculated to an accuracy of first order in the mass ratios for the case of the symmetric rotator.

1. INTRODUCTION

THE formalism of Zemach and Glauber[1] for treating the scattering of low-energy neutrons by chemically bound nuclei in a molecule was applied by them only to the simplest types of molecules as far as the effects of the rotational degrees of freedom are concerned. Procedures for generalizing their results to any type of molecular rotator have been given recently[2] and were used to calculate the distribution of scattered neutrons over energy and angle up to the accuracy of the first quantum-mechanical correction to the classical cross section. The remaining generalized differential cross sections for rotator scattering corresponding to the other types of approximations originally examined by them have now been derived and will be presented here.

In the Fermi pseudo-potential approximation the differential cross section of the entire rotator for a given initial rotational state can be written in the notation of reference 2 as

$$\sigma_i(\vartheta,\epsilon)=(k/2\pi k_0)\sum_{\nu',\nu}\int_{-\infty}^{\infty}e^{-i\epsilon t}\langle\chi_{\nu'\nu}\rangle dt, \qquad (1.1)$$

in which the expectation value in the integrand has the form

$$\langle\chi_{\nu'\nu}\rangle=\langle\psi_i|\,a_{\nu'}a_{\nu}e^{iHt}\exp(i\boldsymbol{\kappa}\cdot\mathbf{b}_{\nu'})e^{-iHt}\exp(-i\boldsymbol{\kappa}\cdot\mathbf{b}_{\nu})\,|\psi_i\rangle.$$

Into this basic expression derived by Zemach and Glauber there has been incorporated by the use of operator techniques the summation over all final states allowed by the conservation laws. The total potential presented to the neutron by the rotator is composed additively of the individual nuclear potentials, so that Eq. (1.1), which is based on the first Born approximation, has the form of a sum of terms which are of two general types. A direct scattering term is one which is attributable to a single nucleus of the rotator while an interference term involves two scattering nuclei. The differential cross section for the direct scattering from a nucleus in the classical or high-energy limit is developed in powers of the ratio of the neutron mass to an effective "rotational mass" of the molecule. The calculation is carried through up to terms of the fourth order in the mass ratio. The expansion of the general expression for the cross section in powers of mass ratios is then discussed and the calculations up to terms of the second order are presented. The very low energy region is considered next and an approximate cross section which is suitable for this limit is derived for the case of the symmetric rotator. When the neutron energy is very low, the number of energetically allowed rotational transitions may be so limited that a direct summing of the partial cross sections for individual transitions is feasible. This alternative procedure is compared with the preceding calculation where the low-energy approximation was applied to a direct scattering term of Eq. (1.1), which contains implicitly the sum over all possible transitions. Finally the portion of the differential cross section which arises from the interference effects due to the presence of more than one scattering nucleus in the rotator and for which no classical approximation exists is treated by means of the mass ratio expansion and the calculation for the symmetric rotator is exhibited up to the first order terms.

2. RÉSUMÉ OF BASIC FORMULAS

The notation to be used here is taken over directly from I. We consider the scattering of a neutron with initial momentum $\mathbf{k}_0$ to final momentum $\mathbf{k}$ by a rotator with fixed center which is in the initial state $|JM\rangle$ having energy E_J, angular momentum J, and component of angular momentum along an axis fixed in space M. The third quantum number required to specify a rotator state is omitted for simplicity in the case of an asymmetric rotator energy eigenstate, where it has no relevant physical significance. Scattering with momentum gain $\boldsymbol{\kappa}=\mathbf{k}-\mathbf{k}_0$ to the neutron corresponds to a certain scattering angle ϑ and energy gain $\epsilon=(2m)^{-1}$

[1] A. C. Zemach and R. J. Glauber, Phys. Rev. **101**, 118, 129 (1956).

[2] H. C. Volkin, Phys. Rev. **113**, 866 (1959). This paper will hereinafter be referred to as I and an equation appearing in it will be designated by the numeral I preceding the equation number.

$\times(k^2-k_0^2)$. The general expression for the differential cross section of the entire rotator is given by Eq. (1.1). The direct scattering term due to the νth nucleus is the term with $\nu'=\nu$, while the two terms involving ν' and ν, with $\nu'\neq\nu$, are the interference terms contributed by the corresponding pair of nuclei. The states which differ only in orientation of the angular momentum vector, i.e., states of different M, are of course degenerate in energy. The cross sections must therefore be averaged over the initial values of M. Also it is sufficient to consider the scattering as spin independent, since the consequences of spin dependence have been treated explicitly by Zemach and Glauber. Then the part of the differential cross section which is due to a single nucleus having position vector $\mathbf{b}$ relative to the center and scattering length a is

$$\sigma_J(\vartheta,\epsilon)=k(2\pi k_0)^{-1}\int_{-\infty}^{\infty}dt\, e^{-i\epsilon t}\langle\chi\rangle_J, \tag{2.1}$$

where the expectation value is given by

$$\langle\chi\rangle_J=a^2(2J+1)^{-1}\sum_{M=-J}^{J}\langle JM|e^{-it(A+B+C)}|JM\rangle. \tag{2.2}$$

The Hermitian operators A, B, C are defined by

$$\begin{aligned}A&=H-E_J,\\ B&=-\boldsymbol{\kappa}\cdot\mathbf{Q}\cdot\mathbf{L}+\tfrac{1}{2}i\mathbf{c}\cdot\boldsymbol{\kappa}\\ &=-\mathbf{L}\cdot\mathbf{Q}^{\dagger}\cdot\boldsymbol{\kappa}-\tfrac{1}{2}i\mathbf{c}\cdot\boldsymbol{\kappa},\\ C&=\tfrac{1}{2}\boldsymbol{\kappa}\cdot\mathbf{R}\cdot\boldsymbol{\kappa}.\end{aligned}$$

The rotator Hamiltonian may be written as $H=\frac{1}{2}\mathbf{L}\cdot\mathbf{G}\cdot\mathbf{L}$, where $\mathbf{L}$ is the angular momentum operator. The tensor $\mathbf{G}$ is the inverse of the moment of inertia tensor, $\mathbf{G}=\mathbf{I}^{-1}$. We further define the tensor quantities $B_{ij}=\epsilon_{imj}b_m$, $\mathbf{R}=\mathbf{B}^{\dagger}\mathbf{G}\mathbf{B}$, $\mathbf{Q}=\mathbf{B}^{\dagger}\mathbf{G}$, and the vector $c_m=b_iG_{im}-(\text{Trace }\mathbf{G})b_m$.

In evaluating the matrix elements (2.2) it will be necessary to express the vector and tensor quantities in terms of components relative to some system of body axes fixed in the rotator, but not necessarily the system of principal axes. When so taken the components of the vector $\mathbf{b}$ and of the tensors given above are constants and commute with the components of $\mathbf{L}$ and $\boldsymbol{\kappa}$ as well as with each other. The momentum transfer vector $\boldsymbol{\kappa}$, which is fixed with respect to space axes, becomes a dynamical variable when seen from the rotating system. The components of $\boldsymbol{\kappa}$ and $\mathbf{L}$ may easily be shown to obey the following commutation relations in this description.

$$[L_i,L_j]=-i\epsilon_{ijk}L_k,\quad [\kappa_i,L_j]=-i\epsilon_{ijk}\kappa_k,\quad [\kappa_i,\kappa_j]=0. \tag{2.3}$$

Let us now designate the set of body axes along which components are being taken by xyz and a set of space axes by XYZ, one of the latter, say Z, being taken for convenience as parallel to $\boldsymbol{\kappa}$ and as the space direction for which M specifies the component of angular momentum. Then a complete set of commuting observables for the rotator is $\mathbf{L}^2$, the component of $\mathbf{L}$ along a body axis, say L_z, and the component of $\mathbf{L}$ along a space axis, say L_Z. The corresponding set of quantum numbers J, K, and M label a complete orthogonal set of basic states $|JKM\rangle$ for the system. An energy eigenstate $|JM\rangle$ can always be expressed as

$$|JM\rangle=\sum_{K=-J}^{J}\alpha_K|JKM\rangle. \tag{2.4}$$

It is to be understood that in the expansion the component K refers to the z axis of the body system chosen to resolve components of the vector and tensor quantities. Then the operation of $\mathbf{L}$ in (2.2) is specified by

$$L_z|JKM\rangle=K|JKM\rangle, \tag{2.5a}$$

$$(L_x\mp L_y)|JKM\rangle=[(J\mp K)(J\pm K+1)]^{\frac{1}{2}}\times|J,K\pm1,M\rangle. \tag{2.5b}$$

In terms of the basic set of states we may write the expectation value (2.2) in the form

$$\langle\chi\rangle_J=a^2\sum_{K,K'}\alpha_K^*\alpha_{K'}\langle\chi\rangle_{JKK'},$$

with

$$\langle\chi\rangle_{JKK'}=(2J+1)^{-1}\textstyle\sum_M\langle JKM|e^{-it(A+B+C)}|JK'M\rangle. \tag{2.6}$$

The Euler angles which specify the orientation of the body axes relative to the space axes are defined as follows: θ and φ are the polar and azimuthal angles, respectively, of the z axis and ψ is the spin angle about this axis. The wave function representatives of the basic set in these variables may be specified by

$$\Psi_{JKM}(\varphi,\mu,\psi)=[(2J+1)/8\pi^2]^{\frac{1}{2}}U^{(J)}{}_{KM}(\varphi,\theta,\psi),$$

where $\mu=\cos\theta$ and $U^{(J)}{}_{KM}$ is the KMth matrix element of the Jth irreducible unitary representation of the rotation group. These matrix elements of the rotation operator are given explicitly as

$$U^{(j)}{}_{km}=\langle jk|U(\varphi,\theta,\psi)|jm\rangle,$$

with

$$U(\varphi,\theta,\psi)=e^{i\psi J_3}e^{i\theta J_2}e^{i\varphi J_3},$$

where the J_i satisfy the usual angular momentum commutation relations and $|jm\rangle$ is an eigenstate of $\mathbf{J}^2$ and J_3. Because of the different conventions which have been used by various authors we mention that the rotation operator U given here transforms an arbitrary state vector $\langle\xi'|$ and arbitrary operator O in the following manner: $\langle\xi'|U(\bar\alpha,\bar\beta,\bar\gamma)$ and $U^{-1}OU$ are the state vector and operator which look in the reference system $\bar X\bar Y\bar Z$ produced by the rotation $(\bar\alpha\bar\beta\bar\gamma)$ from the original reference system XYZ as $\langle\xi'|$ and O do, respectively, in XYZ. In terms of the spherical harmonics

Y_{lm} defined by Condon and Shortley[3] it may be shown that

$$U^{(J)}{}_{0M}(\varphi,\theta,\psi)=[4\pi/(2J+1)]^{\frac{1}{2}}Y_{JM}(\theta,\varphi),$$
$$U^{(J)}{}_{K0}(\varphi,\theta,\psi)=(-1)^K[4\pi/(2J+1)]^{\frac{1}{2}}Y_{JK}(\theta,\psi). \quad (2.7)$$

For certain purposes it will be advantageous to use the principal body axes $\bar{x}\bar{y}\bar{z}$ in which case the tensor $\mathbf{I}$ is diagonal. We write the expansion (2.4) explicitly in this case as

$$|JM\rangle=\sum_{\bar{K}}\bar{\alpha}_{\bar{K}}|J\bar{K}M\rangle, \quad (2.8)$$

where $\bar{K}$ is the component of $\mathbf{L}$ along the principal $\bar{z}$ axis. The form (2.8) is the one generally presented in the literature. It was shown in Appendix C of I that the expansion coefficients are related by the transformation law

$$\alpha_K=\sum_{\bar{K}}\bar{\alpha}_{\bar{K}}U^{(J)}{}_{\bar{K}K}(\alpha,\beta,\gamma), \quad (2.9)$$

where α, β, γ are the Euler angles of the principal axes system relative to the system xyz. The principal axes have the advantage that for a symmetric rotator the states $|J\bar{K}M\rangle$ are themselves the energy eigenstates if the $\bar{z}$ axis is the axis of symmetry, i.e., under these conditions the expansion (2.8) reduces to $\bar{\alpha}_{\bar{K}}=1$, $\bar{\alpha}_{\bar{K}'}=0$ for $\bar{K}'\neq\bar{K}$.

3. CROSS SECTIONS FOR THE DIRECT SCATTERING

For large values of k_0b the term C in the exponential operator of (2.2) dominates. The terms A and B are of order $(\kappa b)^{-2}$ and $(\kappa b)^{-1}$ relative to C. If we write $\lambda=-it$ and the exponential operator as $\exp(\lambda C)f(\lambda)$ with $f(\lambda)=\exp(-\lambda C)\exp\lambda(A+B+C)$, the classical approximation corresponds to replacing $f(\lambda)$ by the unit operator, while the first quantum-mechanical correction consists of retaining terms in the expansion of $f(\lambda)$ up to order $(\kappa b)^{-2}$. These cross sections are derived in I, Sec. 3. The result of the classical approximation can be written as

$$\begin{aligned}\sigma_{\rm cl}(\vartheta,\epsilon)&=2a^2k[\pi(r_1r_2)^{\frac{1}{2}}k_0\kappa^2x]^{-1}K(p)\\ &\qquad\text{for}\quad -\tfrac{1}{2}r_2\kappa^2\leq\epsilon\leq 0,\\ &=2a^2k[\pi(r_1r_2)^{\frac{1}{2}}k_0\kappa^2x]^{-1}qK(q) \quad (3.1)\\ &\qquad\text{for}\quad -\tfrac{1}{2}r_1\kappa^2\leq\epsilon\leq-\tfrac{1}{2}r_2\kappa^2,\\ &=0\quad\text{otherwise,}\end{aligned}$$

where r_1 and r_2 $(r_1\geq r_2>0)$ are the two nonvanishing eigenvalues of $\mathbf{R}$, K is the complete elliptic integral of the first kind, and

$$x^2=1+2\epsilon(r_1\kappa^2)^{-1},$$
$$p^2=q^{-2}=r^{-1}(x^{-2}-1),$$
$$r=r_2(r_1-r_2)^{-1}.$$

The values of r_1 and r_2 are given explicitly in terms of the principal moments of inertia and the components of $\mathbf{b}$ relative to the principal axes in I (3.2).

[3] E. U. Condon and G. H. Shortley, *Theory of Atomic Spectra* (Cambridge University Press, Cambridge, 1935), p. 52.

On introducing the dimensionless variables

$$\Delta=kk_0^{-1}[1+\delta(1-k_0k^{-1}\cos\vartheta)]^{-1},$$
$$\delta=mr_1(1-x^2),$$

we find the differential cross section $\sigma_{\rm cl}(\vartheta)=\int\sigma(\vartheta,\epsilon)d\epsilon$ becomes

$$\sigma_{\rm cl}(\vartheta)=2a^2(r_1r_2)^{\frac{1}{2}}[\pi(r_1-r_2)]^{-1}\Big[\int_0^1 dp\,pK(p)\times\Delta(1+rp^2)^{-\frac{1}{2}}+\int_0^1 dq\,qK(q)\Delta(r+q^2)^{-\frac{1}{2}}\Big]. \quad (3.2)$$

With the help of the relation $kk_0^{-1}=(1+\delta)^{-1}[\delta\cos\vartheta+(1-\delta^2\sin^2\vartheta)^{\frac{1}{2}}]$, we may express Δ in terms of the variable δ alone and can then carry out the power series expansion

$$\Delta=\sum_{n=0}^{\infty}d_n\delta^n.$$

The first few expansion coefficients are

$$d_0=1,\quad d_1=-2(1-\cos\vartheta),$$
$$d_2=\tfrac{1}{2}(1-\cos\vartheta)(5-3\cos\vartheta),\quad d_3=-3(1-\cos\vartheta)^2,$$
$$d_4=\tfrac{1}{8}(1-\cos\vartheta)^2(27-10\cos\vartheta-5\cos^2\vartheta).$$

As a function of p the variable δ has the form $\delta=mr_1rp^2\times(1+rp^2)^{-1}$ while as a function of q it takes the form $\delta=mr_1r(r+q^2)^{-1}$.

If we insert the series expansion of Δ and use the appropriate functional form of δ in the two integrals of Eq. (3.2), we are led to the relation

$$\sigma_{cl}(\vartheta)=(2a^2/\pi)[r(1+r)]^{\frac{1}{2}}\sum_n d_n(-2mr_1r)^n\times[\tfrac{1}{3}\tfrac{1}{5}\cdots(2n+1)^{-1}](\partial/\partial r)^n g(r),$$

with $g(r)=h(r)+r^{-\frac{1}{2}}h(r^{-1})$ where $h(r)=\int_0^1 dq\,qK(q)\times(r+q^2)^{-\frac{1}{2}}$.

In order to evaluate the integral $h(r)$ one can derive from certain differential relations for the complete elliptic integrals the indefinite integral[4]

$$r\int dq\,qK(q)(r+q^2)^{-\frac{1}{2}}=q^2K(q)(r+q^2)^{-\frac{1}{2}}-\Pi(r;q)(r+q^2)^{\frac{1}{2}},$$

where Π is the complete elliptic integral of the third kind. Substituting the desired limits yields

$$h(r)=[r(1+r)]^{-\frac{1}{2}}[\tfrac{1}{2}\pi-\tan^{-1}(r^{\frac{1}{2}})],$$

so that

$$g(r)=\tfrac{1}{2}\pi[r(1+r)]^{-\frac{1}{2}}.$$

We obtain finally the expansion of the classical cross

[4] Integrals similar to this have been calculated in full detail by K. F. Müller, Arch. Electrotech. 17, 336 (1926).

section in powers of the mass ratio mr_1:

$$\sigma_{\rm cl}(\vartheta)/a^2=1+\tfrac{1}{3}(mr_1)(1+2r)(1+r)^{-1}d_1+(1/15)(mr_1)^2\times(3+8r+8r^2)(1+r)^{-2}d_2+(1/35)(mr_1)^3\times(5+18r+24r^2+16r^3)(1+r)^{-3}d_3+(1/315)(mr_1)^4(35+160r+288r^2+256r^3+128r^4)(1+r)^{-4}d_4+\cdots. \quad (3.3)$$

The mass ratio expansion for the general expression (2.2) will now be considered. Following Zemach and Glauber we take the Taylor expansion of the exponential operator and obtain thereby a corresponding expansion of the expectation value in powers of (it) which we write as

$$\langle\chi\rangle_J=\sum_{n=0}^{\infty}e_n(it)^n.$$

This is substituted into (2.1) and then the integration over the variable ϵ is performed. The differential cross section takes the form of a series expansion in powers of the mass ratios (mb_i^2/I_j),

$$\sigma_J(\vartheta)=k_0^{-1}\sum_n\left[(mk^{-1}d/dk)^n k e_n\right]_{k=k_0}. \quad (3.4)$$

In the expansion of $\exp[-it(A+B+C)]$ we see immediately that terms having A all the way to the left or right give no contribution to the expectation values in Eq. (2.2) since $A|JM\rangle=0$. Terms of odd degree in B likewise contribute nothing to the expectation values. It may be seen from Eq. (2.6) that they lead to integrals of the form $(A4)$ which vanish since their integrands are odd. When we retain only contributing terms the expansion of (2.6) to third order in t has the form

$$\langle\chi\rangle_{JKK'}=\delta_{KK'}+(2J+1)^{-1}\sum_M\langle JKM|(-it)C+\tfrac{1}{2}(it)^2(B^2+C^2)-(1/6)(it)^3\times(BAB+CAC+B^2C+CB^2+BCB+C^3)\times|JK'M\rangle. \quad (3.5)$$

One choice of body axes that suggests itself for evaluating the matrix elements (3.5) is the system in which $\mathbf{R}$ is diagonal. The position vector $\mathbf{b}$ is an eigenvector of $\mathbf{R}$ corresponding to the eigenvalue zero, and we take the direction of the z axis along this vector. The components of $\mathbf{Q}$, $\mathbf{G}$, and $\mathbf{c}$ in this system are given in terms of r_1, r_2 and the principal moments of inertia in I, Sec. 3.

The procedure for evaluating the expectation values (2.6) is first to commute the angular momentum components all the way to the right or left of the terms in which they appear. Their operation on the basic states is described by Eqs. (2.5). We then go over to the Euler angle representation. Since no factors dependent on M have been introduced, the average over M can be carried out immediately by using the unitary property of the wave functions. This is illustrated in the Appendix where the resulting integrals are evaluated. Finally the expansion coefficients e_n are inserted into Eq. (3.4). We note that the contributions of C and C^2 in Eq. (3.5) are formally independent of the choice of body axes. This can be seen as follows. Since C does not contain the angular momentum operator, an arbitrary function $f(C)$ does not connect states of different K regardless of the axes system in which components are taken. More precisely we have that

$$(2J+1)^{-1}\sum_M\langle JK'M|f(C)|JKM\rangle=(1/8\pi^2)\delta_{KK'}\int f(C)d\omega, \quad (3.6)$$

with the integral on the right-hand side being taken over all orientations of the rotator. Since C is a scalar invariant, its value for a given orientation of the rotator is independent of the choice of body axes, and therefore the integral is likewise. Using axes which diagonalize $\mathbf{R}$ and the evaluation of integrals in the Appendix, we easily find that the right-hand side of Eq. (3.6) for the case $f(C)=C$ equals $\frac{1}{6}\delta_{KK'\kappa^2}(r_1+r_2)$ and for $f(C)=C^2$ equals $(1/60)\delta_{KK'\kappa^4}(3r_1^2+2r_1r_2+3r_2^2)$. The complete computation to second order in the mass ratios yields

$$\sigma_J(\vartheta)/a^2=1-\tfrac{2}{3}m(r_1+r_2)(1-\cos\vartheta)+(1/30)m^2\times(3r_1^2+2r_1r_2+3r_2^2)(1-\cos\vartheta)(5-3\cos\vartheta)+\tfrac{1}{3}m^2(k_0b)^{-2}\{\tfrac{1}{2}(r_1^2+r_2^2)[J(J+1)-\langle K^2\rangle]+\tfrac{1}{4}(r_1+r_2)^2+b^4(G_{13}^2+G_{23}^2)[\langle K^2\rangle+\tfrac{1}{4}]+\sum_K[(J-K+1)(J+K)]^{\frac{1}{2}}[b^2r_2G_{13}(2K-1)\times\Re(\alpha_K^*\alpha_{K-1})+\tfrac{1}{2}(r_2^2-r_1^2)(J-K+2)^{\frac{1}{2}}\times(J+K-1)^{\frac{1}{2}}\Re(\alpha_K^*\alpha_{K-2})+ib^2r_1G_{23}(2K-1)\Im(\alpha_K^*\alpha_{K-1})]\}, \quad (3.7)$$

where $\langle K^2\rangle=\sum_K\alpha_K^*\alpha_K K^2$ and $\Re$ and $\Im$ denote the real and imaginary parts, respectively.

In the case of the symmetric rotator the symmetry about the principal $\bar{z}$ axis permits placing the nucleus in the plane of the principal $\bar{x}$ and $\bar{z}$ axes. The components of $\mathbf{b}$ relative to the principal axes are then $(b_1,0,b_3)$. Thus the z axis lies in the $\bar{x}\bar{z}$ plane and makes an angle $\beta_0=\tan^{-1}\times(b_1/b_3)$ with the symmetry axis. The Euler angles of the principal axes relative to xyz are seen to be $(0,-\beta_0,0)$. For the energy eigenstate $|J\bar{K}M\rangle$, we have in Eq. (2.8) that

$$\bar{\alpha}_{\bar{K}}=1, \quad \bar{\alpha}_{\bar{K}'}=0 \quad \text{for} \quad \bar{K}'\neq\bar{K}. \quad (3.8)$$

The coefficients α_K are then given by the transformation law (2.9) as

$$\alpha_K=U^{(J)}_{\bar{K}K}(0,-\beta_0,0). \quad (3.9)$$

Formally an average over $\bar{K}$ and $-\bar{K}$ is required, but the cross section for the symmetric rotator is in general even in $\bar{K}$, since the states $|J\bar{K}M\rangle$ and $|J-\bar{K}-M\rangle$ have the same value for the matrix element in Eq. (2.2) and an average over all values of M is taken. That the expression (3.7) for $\sigma_J(\vartheta)$ is even in $\bar{K}$ may be verified explicitly by using the relation

$$U^{(J)}_{-\bar{K}K}(0,-\beta_0,0)=(-1)^{K+\bar{K}}U^{(J)}_{\bar{K}-K}(0,-\beta_0,0).$$

In I the expression for the first quantum correction to the classical cross section was based upon the use of body axes which diagonalize **R**. It was erroneously asserted there (p. 871) that the special case of a symmetric rotator corresponded to the condition (3.8) on the α_K. The coefficients given by (3.9) are instead the generally valid ones. Only when the scattering nucleus lies on the symmetry axis is (3.8) also applicable to the α_K, for then $U^{(J)}_{\bar{K}K}(0,0,0)=\delta_{\bar{K}K}$. The results for the examples of symmetric rotators discussed in I remain unaffected, since for the spherical and linear rotators the axes xyz defined above are also principal axes.

An alternative form for the mass ratio expansion of the cross section may be obtained by using the principal body axes $\bar{x}\bar{y}\bar{z}$ to evaluate the matrix elements (3.5). Again the results will be given to second order in the mass ratios. When the principal body axes are used, **G** is diagonal and in terms of the principal moments of inertia I_i is given by $G_{ii}=I_i^{-1}$. The quantities appearing in the operator B then take the form

$$c_m=b_m(G_{mm}-\text{Trace } \mathbf{G}), \tag{3.10}$$

and

$$\mathbf{Q}=\begin{bmatrix} 0 & b_3I_2^{-1} & -b_2I_3^{-1} \\ -b_3I_1^{-1} & 0 & b_1I_3^{-1} \\ b_2I_1^{-1} & -b_1I_2^{-1} & 0 \end{bmatrix}, \tag{3.11}$$

where the components b_i are, of course, taken with respect to the principal axes. The same procedure used to obtain (3.7) is employed to evaluate the contribution of B^2 in Eq. (3.5).

The alternative expression which is found for the differential cross section by the means described is perhaps a more useful one than Eq. (3.7). The expansion coefficients $\bar{a}_{\bar{K}}$ are the ones generally evaluated in computations of molecular wave functions and they possess the more elementary form (3.8) when the molecules are symmetric. The differential cross section may be written as

$$\begin{aligned}\sigma_J(\vartheta)/a^2 &=1-\tfrac{2}{3}m(\text{Trace } \mathbf{R})(1-\cos\vartheta)+(1/30)m^2 \\ &\times(3r_1^2+2r_1r_2+3r_2^2)(1-\cos\vartheta)(5-3\cos\vartheta) \\ &+\tfrac{1}{3}m^2k_0^{-2}(\tfrac{1}{2}[I_1^{-2}(b_2^2+b_3^2)+I_2^{-2}(b_1^2+b_3^2)] \\ &\times[J(J+1)-\langle\bar{K}^2\rangle]+I_3^{-2}(b_1^2+b_2^2)\langle\bar{K}^2\rangle \\ &+\tfrac{1}{4}[b_1^2(I_2^{-1}+I_3^{-1})^2+b_2^2(I_1^{-1}+I_3^{-1})^2 \\ &+b_3^2(I_1^{-1}+I_2^{-1})^2]+\textstyle\sum_{\bar{K}}[(J-\bar{K}+1)(J+\bar{K})]^{\frac{1}{2}} \\ &\times\{-(2\bar{K}-1)I_3^{-1}b_3[I_1^{-1}b_1\Re(\bar{\alpha}_{\bar{K}}^*\bar{\alpha}_{\bar{K}-1}) \\ &+iI_2^{-1}b_2\Im(\bar{\alpha}_{\bar{K}}^*\bar{\alpha}_{\bar{K}-1})]+\tfrac{1}{2}[I_1^{-2}(b_2^2+b_3^2) \\ &-I_2^{-2}(b_1^2b_3^2)][(J-\bar{K}+2)(J+\bar{K}-1)]^{\frac{1}{2}} \\ &\times\Re(\bar{\alpha}_{\bar{K}}^*\bar{\alpha}_{\bar{K}-2})-iI_1^{-1}I_2^{-1}b_1b_2 \\ &\times[(J-\bar{K}+2)(J+\bar{K}-1)]^{\frac{1}{2}}\Im(\bar{\alpha}_{\bar{K}}^*\bar{\alpha}_{\bar{K}-2})\}). \end{aligned} \tag{3.12}$$

In order to specialize (3.12) to the case of a symmetric rotator, let us take the $\bar{z}$ axis as the axis of symmetry. Then $I_1=I_2$ and the symmetry permits taking $b_2=0$. Furthermore the condition (3.8) is satisfied, so that the summation term vanishes and $\langle\bar{K}^2\rangle=\bar{K}^2$. The resulting expression is even in $\bar{K}$. With $I_1=I_2=I$ and $b^2=b_1^2+b_3^2$ the differential cross section for the symmetric rotator becomes

$$\begin{aligned}\sigma_J(\vartheta)/a^2 &=1-\tfrac{2}{3}(m/II_3)[b^2I_3+b_1^2I+b_3^2I_3](1-\cos\vartheta) \\ &+(1/30)(m/II_3)^2[3b^4I_3^2+2b^2I_3(b_1^2I+b_3^2I_3) \\ &+3(b_1^2I+b_3^2I_3)^2](1-\cos\vartheta)(5-3\cos\vartheta) \\ &+\tfrac{1}{3}(m/k_0II_3)^2\{\tfrac{1}{2}I_3^2(b^2+b_3^2)[J(J+1)-\bar{K}^2] \\ &+I^2b_1^2\bar{K}^2+\tfrac{1}{4}b_1^2(I+I_3)^2+b_3^2I_3^2\}. \end{aligned} \tag{3.13}$$

Two special cases of symmetric rotators are of particular interest. For the spherical rotator we set $I_3=I$ and average over all values of $\bar{K}$, which has the effect of replacing $\bar{K}^2$ by $\frac{1}{3}J(J+1)$, obtaining

$$\begin{aligned}\sigma_J(\vartheta)/a^2 &=1-\tfrac{4}{3}(mb^2/I)(1-\cos\vartheta)+(4/15)(mb^2/I)^2 \\ &\times(1-\cos\vartheta)(5-3\cos\vartheta)+\tfrac{1}{3}(mb/k_0I)^2 \\ &\times[\tfrac{2}{3}J(J+1)+1]. \end{aligned} \tag{3.13a}$$

For the linear rotator we need only set $\bar{K}=0$ and $b_1=0$ in (3.13). The differential cross section for a linear rotator is thus

$$\begin{aligned}\sigma_J(\vartheta)/a^2 &=1-\tfrac{4}{3}(mb^2/I)(1-\cos\vartheta)+(4/15)(mb^2/I)^2 \\ &\times(1-\cos\vartheta)(5-3\cos\vartheta)+\tfrac{1}{3}(mb/k_0I)^2 \\ &\times[J(J+1)+1], \end{aligned} \tag{3.13b}$$

which agrees with the results stated by Zemach and Glauber.

We consider next the region of very low neutron energies where the preceding approximations are inadequate. Here the mass-ratio expansion may be expected either to converge slowly or, for neutron energies less than the rotational level spacing, to diverge. The low-energy approximation is based on the property of Eq. (2.2) that in this limit the term A dominates in the exponential operator. In the approximation to order $(k_0b)^2$ the operator is expanded and terms up to second order in B and first order in C are retained. The desired form of the operator can then be written as

$$\begin{aligned}e^{\lambda(A+B+C)} &=1+\lambda(B+C)+\int_0^\lambda d\lambda'\int_0^{\lambda'}d\lambda''\,Be^{\lambda''A}B \\ &+A(\cdots)+(\cdots)A+O(BC). \end{aligned} \tag{3.14}$$

As explained above the terms with A all the way to the left or right give vanishing contributions in (2.2) and the term linear in B does likewise in the matrix elements (2.6). The matrix elements of C between states $|JKM\rangle$ are known from the previous calculations. In order to handle the integral term explicitly, we now restrict our considerations to the case of a symmetric rotator. The symmetric rotator Hamiltonian and consequently the operator A are diagonal in the basic set of states for which the body-axis component of

angular momentum refers to the symmetry axis. Moreover the eigenvalues are known exactly. Calling the symmetry axis the $\bar{z}$ axis and the common moment of inertia about the other two principal axes I, we write the well-known result

$$H|J\bar{K}M\rangle=E(J,\bar{K})|J\bar{K}M\rangle$$
$$E(J,\bar{K})=\tfrac{1}{2}I^{-1}J(J+1)+\tfrac{1}{2}(I_3^{-1}-I^{-1})\bar{K}^2. \quad (3.15)$$

To find the contribution of the integral term in (3.14) components will be taken in a system of principal axes bearing the notation just given. The symmetry about the $\bar{z}$ axis further allows us to select the $\bar{x}\bar{z}$ plane so as to contain the scattering nucleus, and hence we may set $b_2=0$ in Eqs. (3.10) and (3.11). Since the body axes thus specified are the only ones entering the calculations, we shall for simplicity omit the bar on K which has heretofore been associated with the use of (2.8).

Let us specify the initial state of the rotator by $|JKM\rangle$. In order to evaluate the expectation value $\langle JKM|B\exp(\lambda''A)B|JKM\rangle$, we determine the operation of B on the state vector. Once the vector $B|JKM\rangle$ is known we need only operate on it with the exponential operator using (3.15) and then take the scalar product of the result with the adjoint vector since B is Hermitian. The desired evaluation can be effected in the explicit representation given by the Euler angles $\omega\equiv(\varphi,\theta,\psi)$ of the body axes. The components of $\boldsymbol{\kappa}$ relative to these axes are given by

$$\begin{aligned}\kappa_1&=-\kappa\sin\theta\cos\psi\\&=-(2)^{-\frac{1}{2}}\kappa[U^{(1)}{}_{10}(\omega)-U^{(1)}{}_{-10}(\omega)],\\ \kappa_2&=\kappa\sin\theta\sin\psi\\&=-i(2)^{-\frac{1}{2}}\kappa[U^{(1)}{}_{10}(\omega)+U^{(1)}{}_{-10}(\omega)],\\ \kappa_3&=\kappa\cos\theta=\kappa U^{(1)}{}_{00}(\omega).\end{aligned} \quad (3.16)$$

The operation of B on the symmetric top wave function $N_J U^{(J)}{}_{KM}(\omega)$ is found as follows. Insert (3.16) into one of the forms given for B. Then the products of matrix elements of U are reduced by means of the tabulated Clebsch-Gordan coefficients $(JKlk|JljK+k)$ and the operation of the body-axis components of $\mathbf{L}$ is given by (2.5). The relevant reduction formula[5] is

$$U^{(l)}{}_{k0}(\omega)U^{(J)}{}_{KM}(\omega)=\sum_{j=|J-l|}^{J+l}(JKlk|JljK+k)U^{(j)}{}_{K+k,M}(\omega)\times(JMl0|JljM). \quad (3.17)$$

After performing the computations outlined and averaging over M, we collect the contributions of the various terms in (3.14) to the expectation value (2.2) and obtain finally for the scattering cross section of a symmetric rotator in this approximation

$$\begin{aligned}&\sigma_{JK}(\vartheta,\epsilon)/a^2\\&=kk_0^{-1}[1-\tfrac{1}{3}\kappa^2b^2+\tfrac{1}{3}\kappa^2b_3^2J^{-1}(J+1)^{-1}K^2]\delta(\epsilon)\\&\quad+\tfrac{1}{3}kk_0^{-1}\kappa^2b_3^2(2J+1)^{-1}\{(J+1-K)(J+1+K)\\&\quad\times(J+1)^{-1}\delta[\epsilon+\Delta(J+1,K)]\\&\quad+(J-K)(J+K)J^{-1}\delta[\epsilon+\Delta(J-1,K)]\}\\&\quad+(1/12)kk_0^{-1}\kappa^2b_1^2([(J+1)(2J+1)]^{-1}\\&\quad\times\{(J+1+K)(J+2+K)\delta[\epsilon+\Delta(J+1,K+1)]\\&\quad+(J+1-K)(J+2-K)\delta[\epsilon+\Delta(J+1,K-1)]\}\\&\quad+[J(J+1)]^{-1}\{(J-K)(J+1+K)\\&\quad\times\delta[\epsilon+\Delta(J,K+1)]+(J+K)(J+1-K)\\&\quad\times\delta[\epsilon+\Delta(J,K-1)]\}+[J(2J+1)]^{-1}\\&\quad\times\{(J-K)(J-1-K)\delta[\epsilon+\Delta(J-1,K+1)]\\&\quad+(J+K)(J-1+K)\delta[\epsilon+\Delta(J-1,K-1)]\}),\end{aligned} \quad (3.18)$$

where the rotational level spacing is written as $\Delta(J_1,K_1)=E(J_1,K_1)-E(J,K)$. Writing $\rho=-(2m/k_0^2)\Delta(J_1,K_1)$ we have for the transition $(J,K)\rightarrow(J_1,K_1)$

$$kk_0^{-1}\kappa^2=2k_0^2(1+\rho)^{\frac{1}{2}}[1+\tfrac{1}{2}\rho-(1+\rho)^{\frac{1}{2}}\cos\vartheta]. \quad (3.19)$$

The condition $|\rho|\ll1$ holds when the mass ratios are sufficiently small. We can expand the right-hand side of Eq. (3.19) in powers of ρ and obtain thereby a mass ratio expansion of the low-energy cross section (3.18). Retaining terms to second order in ρ yields the first, second, and fourth of the four terms presented in the more general expansion (3.13). This agrees with the observation of Zemach and Glauber that the mass ratio expansion of the low-energy approximation contains the terms which dominate at low energies in the more general expansion (3.5).

It is of interest to consider the explicit summing of the partial cross sections for individual rotational transitions. The procedures involved will be described for the symmetric rotator and the very low energy case will then be compared to the preceding calculation. We begin with the expression for the differential cross section of the scattering process, in which the rotator undergoes a transition from the initial state ψ_i to the final state ψ_f,

$$\sigma_{fi}(\vartheta)=\sum_{\nu',\nu}a_{\nu'}a_\nu(k/k_0)M_{\nu'}{}^*M_\nu, \quad (3.20)$$

where the sum is taken over all nuclei of the rotator and

$$M_\nu=\langle\psi_f|\exp(-i\boldsymbol{\kappa}\cdot\mathbf{b}_\nu)|\psi_i\rangle.$$

The complete cross section for a given initial state is the sum of the partial cross sections (3.20) over all final states allowed by the conservation laws. The component M of the rotator's angular momentum $\mathbf{L}$ along $\boldsymbol{\kappa}$ remains unchanged during a collision, since the change in the neutron's orbital angular momentum is perpendicular to $\boldsymbol{\kappa}$. Hence, with K again designating the component of $\mathbf{L}$ along the symmetry axis, we require the matrix elements for the transitions (J,K)

[5] See, for example, A. R. Edmonds, *Angular Momentum in Quantum Mechanics* (Princeton University Press, Princeton, 1957), p. 60.

$\rightarrow (J+n, K+k)$, which we write as

$$M_{nk}=\langle J+n\, K+k\, M|\exp(-i\boldsymbol{\kappa}\cdot\mathbf{b})|JKM\rangle. \quad (3.21)$$

The same system of principal axes as in the low-energy calculation will now be used, and we call θ_0 the polar angle of $\mathbf{b}$ with the Z axis or $\boldsymbol{\kappa}$ and β_0 the angle which $\mathbf{b}$ makes with the symmetry $\bar{z}$ axis. Recalling that the principal $\bar{x}\bar{z}$ plane may be chosen to contain the nucleus, we have $\beta_0=\tan^{-1}(b_1/b_3)$. Now consider the expansion of the exponential in (3.21) in Legendre polynomials $P_l(\cos\theta_0)$. The addition theorem enables us to express each P_l in terms of the polar and azimuthal angles of $\mathbf{b}$ and $\boldsymbol{\kappa}$ relative to the body axes, namely $(\beta_0,0)$ and $(-\theta,-\psi)$, respectively. Combining these two developments gives

$$\exp(-i\boldsymbol{\kappa}\cdot\mathbf{b})=\sum_{l=0}^{\infty}[4\pi(2l+1)]^{\frac{1}{2}}(-i)^l j_l(\kappa b) \times\sum_{k=-l}^{l}Y_{lk}(\beta_0,0)U^{(l)}{}_{k0}(\omega). \quad (3.22)$$

The matrix elements (3.21) can be evaluated in the Euler angle representation by means of the reduction formula (3.17). It is seen that each higher l value in (3.22) introduces larger values of $|J+n|$ in the resolution of $\exp(-i\boldsymbol{\kappa}\cdot\mathbf{b})U^{(J)}{}_{KM}$. Of course, only energetically allowed transitions can actually occur.

The nature of the low-energy approximation is revealed through the asymptotic behavior of the spherical Bessel functions for small arguments:

$$j_l(x)\approx[1\cdot3\cdots(2l+1)]^{-1}x^l[1-\tfrac{1}{2}(2l+3)^{-1}x^2].$$

Since the cross section for a direct scattering collision ($\nu'=\nu$) involves the square of the magnitude of the matrix elements (3.21), the approximation to order $(\kappa b)^2$ is a consequence of retaining terms up to $l=2$ in (3.22). In fact, this approximation gives precisely the cross section (3.18). For example, contributions to the elastic scattering come from the $l=0,1,2$ and $k=0$ terms with the result that

$$(2J+1)^{-1}\sum_{M=-J}^{J}|M_{00}|^2=1-\tfrac{1}{3}\kappa^2b^2+\tfrac{1}{3}\kappa^2b_3^2J^{-1}(J+1)^{-1}K^2.$$

The inelastic terms in (3.18) come from the $l=1$ and $k=-1,0,1$ terms.

4. INTERFERENCE SCATTERING

The part of the rotator cross section due to interference scattering involving nuclei 1 and 2 is obtained by replacing the single expectation value in Eq. (2.1) by the pair $\langle\chi_{12}\rangle_J+\langle\chi_{21}\rangle_J$. If $\mathbf{b}_{12}=\mathbf{b}_1-\mathbf{b}_2$, the first expectation value is given by

$$\langle\chi_{12}\rangle_J=a_1a_2(2J+1)^{-1}\textstyle\sum_M\langle JM|\exp(i\boldsymbol{\kappa}\cdot\mathbf{b}_{12}) \times\exp[-it(A+B_2+C_2)]|JM\rangle, \quad (4.1)$$

where the subscript 2 on the operators B and C indicates that they are taken with reference to nucleus 2. In the second expectation value the roles of 1 and 2 are interchanged. We shall again employ the technique of expanding the expectation values in powers of (it) and then applying Eq. (3.4).

The case of a symmetric rotator in the initial state $|J\bar{K}M\rangle$ will be treated to first order accuracy in the mass ratios. For taking components we use the system of principal axes in which $\bar{z}$ is the symmetry axis and the $\bar{x}\bar{z}$ plane is parallel to $\mathbf{b}_{12}$. Hereafter the bar on K will be omitted. We let γ_0 be the angle which $\mathbf{b}_{12}$ makes with the $\bar{z}$ axis and $\mathbf{d}=\mathbf{b}_{12}$. In the expressions to come the notation will be simplified if we write components in this system as follows: $\mathbf{d}=(d_i)$, $\boldsymbol{\kappa}=(\bar{\kappa}_i)$, $\mathbf{b}_1=(u_1,u_2,u_3)$, and $\mathbf{b}_2=(v_1,v_2,v_3)$. In (4.1) the quantities $\mathbf{c}$ and $\mathbf{Q}$ are obtained from (3.10) and (3.11), respectively, by inserting for b_i the components of $\mathbf{b}_2$. Similarly the tensor $\mathbf{R}$ has components $R_{ii}=v_j^2I_k^{-1}+v_k^2I_j^{-1}$, $R_{ij}=-v_iv_jI_k^{-1}$, $i\neq j\neq k$. Throughout we set $I_1=I_2=I$. Then from the unitary property of the $U^{(J)}{}_{KM}$ we obtain

$$\begin{aligned}
&(2J+1)^{-1}\textstyle\sum_M\langle JKM|\exp(i\boldsymbol{\kappa}\cdot\mathbf{d})|JKM\rangle\\
&\quad=(1/8\pi^2)\int\exp(i\boldsymbol{\kappa}\cdot\mathbf{d})d\omega,\\
&(2J+1)^{-1}\textstyle\sum_M\langle JKM|\exp(i\boldsymbol{\kappa}\cdot\mathbf{d})B_2|JKM\rangle\\
&\quad=(1/8\pi^2)\int\exp(i\boldsymbol{\kappa}\cdot\mathbf{d})[-Q_{13}K\bar{\kappa}_1-Q_{23}K\bar{\kappa}_2+\tfrac{1}{2}ic_m\bar{\kappa}_m]d\omega,\\
&(2J+1)^{-1}\textstyle\sum_M\langle JKM|\exp(i\boldsymbol{\kappa}\cdot\mathbf{d})C_2|JKM\rangle\\
&\quad=(1/8\pi^2)\int\exp(i\boldsymbol{\kappa}\cdot\mathbf{d})\tfrac{1}{2}R_{mn}\bar{\kappa}_m\bar{\kappa}_nd\omega.
\end{aligned} \quad (4.2)$$

In (4.2) the integrals are taken over all orientations of the rotator.

The integrals occurring in (4.2) can be expressed as a linear combination of integrals which are evaluated in the Appendix by the following transformation of variables in the integrands. The transformation corresponds to a rotation from the original principal axes to the system of body axes in which $\mathbf{d}$ is parallel to the new z axis, i.e., to a rotation through the angle $\gamma_0=\tan^{-1}(d_1/d_3)$ about the $\bar{y}$ axis.

$$\begin{aligned}
\bar{\kappa}_1&=\kappa_1\cos\gamma_0+\kappa_3\sin\gamma_0,\\
\bar{\kappa}_2&=\kappa_2,\\
\bar{\kappa}_3&=-\kappa_1\sin\gamma_0+\kappa_3\cos\gamma_0.
\end{aligned} \quad (4.3)$$

For example, the use of the transformation (4.3) in the second integral of (4.2) yields in the notation of the Appendix

$$(2J+1)^{-1}\textstyle\sum_M\langle JKM|\exp(i\boldsymbol{\kappa}\cdot\mathbf{d})B_2|JKM\rangle =(1/8\pi^2)[(-Q_{13}K+\tfrac{1}{2}ic_1)\sin\gamma_0+\tfrac{1}{2}ic_3\cos\gamma_0]I(001).$$

After evaluating the integrals in (4.2) we then have $\langle \chi_{12} \rangle_J$ to the desired accuracy and it can be expressed in terms of j_0 and j_1 alone by means of the relation $j_2(x)=3x^{-1}j_1(x)-j_0(x)$. The corresponding expression for $\langle \chi_{21} \rangle_J$ is obtained by interchanging 1 and 2 in the previous result. Adding the two expectation values and averaging over $+K$ and $-K$, we obtain finally from Eq. (3.4)

$$\sigma_{\text{int}}^{(1,2)}(\vartheta)/a_1a_2$$

$$=2j_0(\kappa d)-\frac{m}{k_0^2}\frac{\partial}{\partial k}\left\{\frac{k\kappa^2}{Id^2}(\mathbf{b}_1\times\mathbf{b}_2)^2 j_0(\kappa d)\right.$$

$$+\frac{k\kappa}{d}\left[\left(\frac{1}{I}+\frac{1}{I_3}\right)(\mathbf{b}_1\cdot\mathbf{b}_2)-\frac{3}{Id^2}(\mathbf{b}_1\times\mathbf{b}_2)^2\right]j_1(\kappa d)$$

$$+\frac{k\kappa}{2d}\left(\frac{1}{I}-\frac{1}{I_3}\right)\left[2u_3v_3 j_1(\kappa d)+(u_2^2+v_2^2)\frac{d_1^2}{d}\right.$$

$$\left.\left.\times\left(\frac{3}{d}j_1(\kappa d)-\kappa j_0(\kappa d)\right)\right]\right\}_0. \quad (4.4)$$

APPENDIX

After the angular momentum components are allowed to operate upon the basic states in the expectation value (3.5), there remains a collection of terms each containing the expectation value of a product of the form $\kappa_1^{n_1}\kappa_2^{n_2}\kappa_3^{n_3}$, where the n_i are integers. The κ_i are the components with respect to a set of body axes xyz fixed in the rotator of a quantity κ directed along the Z axis fixed in space. Going over to the representation in the Euler angles $\omega\equiv(\varphi,\theta,\psi)$ of the body axes we have

$$\frac{1}{(2J+1)}\sum_{M=-J}^{J}\langle JKM|\kappa_1^{n_1}\kappa_2^{n_2}\kappa_3^{n_3}|JK'M\rangle$$

$$=\frac{1}{8\pi^2}\sum_{M=-J}^{J}\int d\omega\, U^{(J)}_{KM}{}^*(\omega)U^{(J)}_{K'M}\times(\omega)\kappa_1^{n_1}\kappa_2^{n_2}\kappa_3^{n_3}. \quad (A1)$$

where $d=\omega d\varphi d\psi\sin\theta d\theta$ and the integration extends over all orientations of the body. The sum over M can be carried out immediately with the help of the unitary property of the matrix $U^{(J)}$. The right-hand side of Eq. (A1) becomes $(1/8\pi^2)\delta_{KK'}J(n_1n_2n_3)$ with

$$J(n_1n_2n_3)=\int \kappa_1^{n_1}\kappa_2^{n_2}\kappa_3^{n_3}d\omega. \quad (A2)$$

Expressing the components in terms of the Euler angles as in Eq. (3.16) and letting $n=n_1+n_2+n_3$, we can write the integral J in the product form

$$J(n_1n_2n_3)=\kappa^n G(n_1n_2)F(n_1n_2n_3),$$

where

$$G(n_1n_2)=2\pi(-1)^{n_1}\int_0^{2\pi}d\psi\,(\cos\psi)^{n_1}(\sin\psi)^{n_2}=\frac{\pi[1+(-1)^{n_1}][1+(-1)^{n_2}]\Gamma[\frac{1}{2}(n_1+1)]\Gamma[\frac{1}{2}(n_2+1)]}{\Gamma[\frac{1}{2}(n_1+n_2+2)]}, \quad (A3)$$

and

$$F(n_1n_2n_3)=\int_0^{\pi}d\theta\,(\cos\theta)^{n_3}(\sin\theta)^{n_1+n_2+1}=[1+(-1)^{n_3}]\Gamma[\tfrac{1}{2}(n_3+1)]\Gamma[\tfrac{1}{2}(n_1+n_2+2)]/2\Gamma[\tfrac{1}{2}(n+3)].$$

Combining these results gives

$$J(n_1n_2n_3)=\tfrac{1}{2}\pi\kappa^n\left\{\prod_{i=1}^{3}[1+(-1)^{n_i}]\Gamma[\tfrac{1}{2}(n_i+1)]\right\}\Big/\Gamma[\tfrac{1}{2}(n+3)].$$

The expectation values encountered in Sec. 4 led to integrals of the type

$$I(n_1n_2n_3)=\int e^{id\kappa_3}\kappa_1^{n_1}\kappa_2^{n_2}\kappa_3^{n_3}d\omega, \quad (A4)$$

which can be expressed in the form

$$I(n_1n_2n_3)=\kappa^n G(n_1n_2)H(n_1n_2n_3), \quad (A5)$$

$$H(n_1n_2n_3)=\int_{-1}^{1}d\mu\, e^{id\kappa\mu}(1-\mu^2)^{(n_1+n_2)/2}\mu^{n_3}. \quad (A6)$$

Since $G(n_1n_2)$ vanishes unless n_1 and n_2 are both even, we need only consider the case $\frac{1}{2}(n_1+n_2)$ equal to an integer. When in Eq. (A6) we raise $(1-\mu^2)$ to an integral power, each term contains an even power of μ. A typical term, say μ^{2m}, yields an expression of the type

$$\int_{-1}^{1}d\mu\left[\sum_{l=0}^{2m+n_3}(2l+1)i^l j_l(\kappa d)P_l(\mu)\right]\mu^{2m+n_3}. \quad (A7)$$

The sum in (A7) is effectively over only even or only odd values of l depending on whether n_3 is an even or odd integer, respectively, because $P_l(-\mu)=(-1)^l P_l(\mu)$. The integrals in (A7) are all special cases of a general integral formula.[6] The particular integrals (A6) required to derive Eq. (4.4) are $H(000)=2j_0(\kappa d)$, $H(001)=2ij_1(\kappa d)$, $H(200)=H(020)=\frac{4}{3}[j_0(\kappa d)+j_2(\kappa d)]$ and $H(002)=\frac{2}{3}[j_0(\kappa d)-2j_2(\kappa d)]$.

[6] Bateman Manuscript Project, *Higher Transcendental Functions* (McGraw-Hill Book Company, Inc., New York, 1953), Vol. 1, p. 171, Eq. (23).